MODELING OF SMOLDERING CELLULOSIC MATERIALS-
EVAPORATION AND PYROLYSIS PROCESSES

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INTRODUCTION
Over 1600 people die each year [Miller, 1991] from fires started by smoking materials (cigarettes, matches, etc.), and many times that number are hurt and/or disfigured; most of those fires are established in upholstered furniture. As a result, Congress passed the Cigarette Safety Act of 1984. One of the tasks under the Act was to model mathematically the behavior of upholstered furniture and the cigarette, when a smoldering cigarette is dropped onto it. To do this, the heating of the substrate when subjected to a moving heat source must first be accurately modeled, and a criterion established for its ignition. In order to examine how changing one or more properties of the cigarette will influence its ignition propensity, it is also necessary to understand the behavior of a smoldering cigarette. This includes knowing how its external heat flux and burning velocity depend upon its physical and/or chemical properties.

Considerable effort has been expended in the study of the burning cellulosic material such as tobacco etc.. Egerton et al. [1963] studied the smoldering combustion in cigarettes. From the data of various experiments, they explained several aspects of the mechanism of smoldering. A theoretical and experimental investigation of the smoldering mechanism of a cylindrical cellulosic rod was carried out by Moussa et al. [1976]. They proposed a simple steady-state, 1-dimensional model of a burning cellulosic rod. Based on a postulated mechanism of smoldering, Muramatsu et al. [1979] developed one-dimensional model of the pyrolysis/distillation zone. Their model contains four general pyrolysis reactions, one distillation process and combined conductive and radiative heat transfer from the combustion zone.

The purpose of this paper is to present the results of a study using numerical techniques to compute the static burn rate, mass burn rate, heat flux and the amount of heat released in the natural smoldering cigarette. The study was made on cigarettes containing flue-cured and burley tobaccos since physical properties and kinetic data are readily available [Muramatsu et al. 1979].
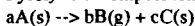
MATHEMATICAL MODEL
A cigarette generally includes a filter attached to the end of the tobacco rod. The rod is a packed column of approximately 1 g of shredded tobacco, generally 8 mm in diameter and 70 mm long, wrapped in a thin porous paper. The shreds are nonuniformly packed in the tobacco rod which contains about 70 - 85 % void space.

Smoldering is a non-flaming combustion mode, characterized by thermal degradation and charring of the virgin tobacco, evolution of smoke, and emission of a visible glow. The temperature in the burning zone increases to the ignition temperature, and the temperature gradients are directly correlated to the basic processes which take place in the cigarette (i.e. distillation, pyrolysis, and combustion) and affect the absolute density [Baker, 1979] of the rod in the burning zone.

During natural burning the oxygen transport to the surface is restricted and the peripheral region with its large heat losses cannot maintain rapids surface oxidation. Muramatsu et al. have developed a model of the evaporation-pyrolysis processes with the following assumptions:
1) The solid phase and the gas phase inside the burning tobacco are the same temperature.
2) Heat loss from the outer surface of the element is caused by free convection and radiation.
3) Heat transfer inside the cigarette column is caused by thermal conduction characterized by a effective thermal conductivity.

Pyrolytic decomposition of tobacco can be expressed by the following simplified equation;
aA(s) --> bB(g) + cC(s)
The virgin tobacco and its water content are gradually consumed to form smoke, water vapor, and a residual char with final density ρ_f. In the steady state of combustion, the temperature is raised by the heat transferred from the burning zone. The temperature distribution of the tobacco column depends upon the thermal properties of the cigarette such as the effective thermal conductivity, specific heat and thermal diffusivity. The total density of the burning tobacco is given by

$$\rho_t = \rho_v + \rho_c + \rho_w \qquad (1)$$

where ρ is density, and the subscripts t, v, c, and w stand for total, unreacted tobacco, carbonaceous residue, and water, respectively. The conversion of virgin tobacco can be expressed by

$$\frac{\partial \rho_v}{\partial t} = \sum_{i=1}^{4} \frac{\partial \rho_{vi}}{\partial t} \tag{2}$$

and then the individual Arrhenius forms:

$$\frac{\partial \rho_{vi}}{\partial t} = -A_i \exp\left(\frac{-E_i}{RT}\right)\left(\frac{\rho_{vi}}{\rho_{vi}^o}\right)^n \rho_{vi}^o \tag{3}$$

and the char density is given by

$$\frac{\partial \rho_c}{\partial t} = -\frac{\rho_f}{\sum_{i=1}^{4} \rho_{vi}^o} \frac{\partial \rho_v}{\partial t} \tag{4}$$

where superscript o is the initial state. The loss of tobacco moisture from a tobacco rod is assumed to involve both the conversion of moisture to a water vapor as well as mass transfer of the moisture out of the tobacco rod. The evaporation rate of the water from tobacco can be expressed by the empirical equation,

$$\frac{\partial w}{\partial t} = -\left(\frac{S}{w}\right)\exp\left(\frac{-\theta}{T}\right)(w - w_{eq})^\beta \tag{5}$$

where w is water content in tobacco, S is surface area of a tobacco lamina, θ and β are empirical constants, and subscript eq is equilibrium state. The pyrolysis reaction of virgin tobacco in the region where water evaporation takes place is slow, and can be considered to be negligible. Thus

$$\frac{\partial \rho_w}{\partial t} = -N_a \alpha \exp\left(\frac{-\theta}{T}\right)(w - w_{eq})^\beta = \sum_{i=1}^{4} \rho_{vi}^o \frac{\partial w}{\partial t} \tag{6}$$

where N_t is total surface area of tobacco shreds per unit volume of a cigarette, α is experimental constant, and w_{eq} is related to the water vapor pressure, p_w, by

$$w_{eq} = \frac{p_w/p_{ws}}{a + b\left(p_w/p_{ws}\right) - c\left(p_w/p_{ws}\right)^2} \tag{7}$$

The saturated vapor pressure of water, p_{ws}, can be expressed by Calingart's equation [Calingert and Davis, 1925] as follows;

$$\log p_{ws} = 7.991 - \frac{1687}{T - 43} \tag{8}$$

The mass balance equation for the water vapor pressure, p_w, inside the tobacco rod is

$$\frac{\partial}{\partial t}\left(\frac{p_w}{RT}\right) = \frac{\partial}{\partial z}\left\{D_z \frac{\partial}{\partial z}\left(\frac{p_w}{RT}\right)\right\} - \frac{2D_r}{\Phi r \delta RT}\left(p_w - p_{w\infty}\frac{T}{T_\infty}\right) - \frac{\sum_{i=1}^{4} \rho_{vi}^o}{\Phi m}\frac{\partial w}{\partial t} \tag{9}$$

where the first term of left hand side is the net rate of accumulation of water vapor, the first term of right hand side (rhs) is the rate of accumulation water vapor by diffusion, the second term of rhs is the rate of loss of water vapor by diffusion through a cigarette paper of thickness, δ, and the last term is the rate of evaporation of water from the tobacco.

The heat balance equation for the element is given by
$$\frac{\partial(H_v\rho_v + H_c\rho_c + H_w\rho_w)}{\partial t} = \frac{\partial}{\partial z}\left(K_e \frac{\partial T}{\partial z}\right) + Q_p \frac{\partial \rho_v}{\partial t} + Q_w \frac{\partial \rho_w}{\partial t} - \frac{2}{r}\left\{h(T - T_\infty) + \sigma \varepsilon_s(T^4 - T_\infty^4)\right\} \tag{10}$$

where the thermal conductivity, K_e, depends upon the void fraction, ϕ and the temperature, T.

$$K_e = (1 - \phi^{2/3})K_s + \phi^{1/3}(1 + \frac{2}{3}h_r D_p / K_g)K_g \tag{11}$$

where
$$h_r = 5.422 x 10^{-12} \varepsilon_s T^3$$

The cigarette weight after t time is;

$$M(t) = u\pi r^2 \int_0^n \rho_e(t, r, \%moisture, ...)dt \tag{12}$$

The heat flux is then given by;

$$q = \frac{1}{x}\int_0^x \frac{2}{r}\left[h(T - T_\infty) + \sigma \varepsilon_s(T^4 - T_\infty^4)\right]dx \tag{13}$$

and the initial and boundary conditions are;

$$T = T_\infty @ x = -\infty$$

$$T = T_o @ x = x_o$$

$$\left(\frac{dT}{dx}\right)_{x=x_o} = \frac{u}{K_e}(T - T_\infty)(\rho_{vo}C_{pvo} + \rho_{wo}C_{pwo}) \qquad (14)$$

$$\rho_{ao} = \frac{M_o}{V}, \rho_{wo} = \rho_{ao}\frac{w_o}{1+w_o}, \rho_{co} = 0.0, \rho_{vo} = \rho_{ao} - \rho_{wo}$$

w_o refers to the moisture content in the tobacco. The values of physical parameters used to solve the simultaneous differential equations can be obtained elsewhere [Muramatsu et al., 1979]. Then, the set of simultaneous differential equations can be solved numerically by the LSODE.

RESULTS AND DISCUSSIONS
In this section, we examine the factors affecting the static burn rate, the mass burn rate, heat flux and the heat released at the boundary by convection and radiation. The results are expected to provide a tool for understanding the mechanism of smoldering and controlling the physical parameters in the design of cigarette.

The mass burn rate (MBR), static burn rate (SBR), heat flux and heat released shown in Table 1 as a function of cigarette moisture at constant circumference and initial density. The analysis reveals that the SBR and MBR decrease with increased cigarette moisture content and are linear functions within the range of 10 to 15 % moisture. Thus, increased moisture reduces the rate of combustion due to the extra heat needed to vaporize water from the tobacco. The approximate value of heat flux regardless of moisture content are 0.327 and 0.177 cal/cm^2 sec for burley and flue-cured, respectively. The total heat released from the cigarette rod, neglecting the contribution from the paper is a function of the moisture content of the rod. The calculated heat released values at 12 % moisture are 1734 cal for burley and 1344 cal for flue-cured tobaccos. These values agree well with the results of Muramatsu et al.[1979]. Therefore, an increase in the tobacco moisture content causes a decrease in the static burn rate, but an increase in the total heat released.

The packing density of the cigarette has an effect on the SBR and MBR. Table 2 shows the typical smoldering speed calculated for a cigarette containg burley and flue-cured tobaccos and indicate that increasing the density at constant moisture and circumference causes the SBR to decrease. However, results show that the increase of the rod density appears to increase the MBR only slighty.

Table 3 summarizes the effect of rod circumference on the SBR and MBR. The results show that the MBR increase as circumference increases.

CONCLUSIONS
A mathematical model of the natural smoldering of cellulosic material is presented. The following conclusions can be drawn;
1) A simple interpretation of the calculation is that the variations in tobacco moisture content, rod densuty and circumferences can explain variations in SBR, MBR, heat flux and total heat released.
2) The calculation illustrates that the circumference of the cigarette is the major physical factor affecting MBR, while rod densuty strongly affects the SBR, heat flux, and heat released.
3) A quantitative relationship between these parameters and the MBR, SBR, and heat flux has been developed. The results may be a useful predictive tool for use in cigarette design.

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Table 1. Calculated values of moisture content vs. SBR, MBR, and heat released.

A. Burley

Moisture content (%)	Static burn rate (10^{-3} cm/sec)	Mass burn rate (mg/min)	Heat released (cal)
10.0	6.497	74.178	1644.1
10.9	6.330	72.001	1691.7
12.0	6.112	69.218	1734.5
13.0	5.905	66.590	1797.4
14.0	5.692	63.951	1865.2
15.0	5.479	61.311	1937.6

B. Flue-cured

Moisture content (%)	Static burn rate (10^{-3} cm/sec)	Mass burn rate (mg/min)	Heat released (cal)
11.0	4.676	60.365	1308.7
12.0	4.563	58.731	1344.4
13.1	4.430	56.813	1387.9
14.0	4.318	55.220	1425.8
15.0	4.190	53.406	1471.1
16.0	4.060	51.587	1519.3

Table 2. Initial density effect on the SBR, MBR, and heat released.

Initial density (g/cc)	Static burn rate (10^{-3} cm/sec)		Mass burn rate (mg/min)		Heat released (cal)	
	flue-cured	burley	flue-cured	burley	flue-cured	burley
0.213	5.901	7.630	52.270	67.933	1057.2	1424.5
0.228	5.520	7.142	53.459	69.479	1133.3	1489.4
0.313	3.970	5.149	58.149	75.548	1552.9	2053.0
0.341	3.620	4.709	59.143	76.845	1693.5	2242.0
0.370	3.340	4.338	59.981	77.924	1838.4	2431.2

Table 3. Circumference effect on the MBR and heat released.

Circumference (cm)	Mass burn rate (mg/min)		Heat released (cal)	
	flue-cured	burley	flue-cured	burley
2.10	35.888	46.197	1563.6	1788.3
2.20	40.544	51.886	1511.8	1758.0
2.30	45.468	58.011	1466.8	1711.9
2.40	50.662	64.401	1431.3	1702.8
2.512	56.813	72.001	1387.9	1691.7
2.60	61.867	78.244	1371.2	1662.2
2.70	67.868	85.669	1363.4	1656.2
2.80	74.129	93.420	1344.6	1637.9